



#10

1

SEQUENCE LISTING

<110> WALKER, SUZANNE

<120> CRYSTALS OF THE ESCHERICHIA COLI MEMBRANE-ASSOCIATED
GLYCOSYLTRANSFERASE (MURG) PROTEIN, ATOMIC COORDINATES
AND THREE DIMENSIONAL STRUCTURES THEREOF, ATOMIC
COORDINATES AND THREE DIMENSIONAL STRUCTURES OF
BINDING DOMAINS THEREOF, IMAGES THEREOF, AND METHODS
OF CRYSTALLIZING MURG PROTEINS, MODELS OF UDP-
GLYCOSYLTRANSFERASES, MURG PROTEINS AND BINDING SITES,
METHODS OF MAKING MODELS, METHODS OF USING MODELS OF
MURG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MURG
PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

<130> 4555-105

<140> 09/829,275

<141> 2001-04-09

<160> 8

<170> PatentIn Ver. 2.1

<210> 1

<211> 364

<212> PRT

<213> Escherichia coli

<400> 1

Met Met Ser Gly Gln Gly Lys Arg Leu Met Val Met Ala Gly Gly Thr
1 5 10 15

Gly Gly His Val Phe Pro Gly Leu Ala Val Ala His His Leu Met Ala
20 25 30

Gln Gly Trp Gln Val Arg Trp Leu Gly Thr Ala Asp Arg Met Glu Ala
35 40 45

Asp Leu Val Pro Lys His Gly Ile Glu Ile Asp Phe Ile Arg Ile Ser
50 55 60

Gly Leu Arg Gly Lys Gly Ile Lys Ala Leu Ile Ala Ala Pro Leu Arg
65 70 75 80

Ile Phe Asn Ala Trp Arg Gln Ala Arg Ala Ile Met Lys Ala Tyr Lys
85 90 95

Pro Asp Val Val Leu Gly Met Gly Gly Tyr Val Ser Gly Pro Gly Gly
100 105 110

Leu Ala Ala Trp Ser Leu Gly Ile Pro Val Val Leu His Glu Gln Asn
115 120 125

Gly Ile Ala Gly Leu Thr Asn Lys Trp Leu Ala Arg Ile Ala Thr Lys
130 135 140

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TECH CENTER 1600/2900

Val Met Gln Ala Glu Pro Gly Ala Phe Pro Asn Ala Glu Val Val Gly
 145 150 155 160
 Asn Pro Val Arg Thr Asp Val Leu Ala Leu Pro Leu Pro Gln Gln Arg
 165 170 175
 Leu Ala Gly Arg Glu Gly Pro Val Arg Val Leu Val Val Gly Gly Ser
 180 185 190
 Gln Gly Ala Arg Ile Leu Asn Gln Thr Met Pro Gln Val Ala Ala Lys
 195 200 205
 Leu Gly Asp Ser Val Ile Ile Trp His Gln Ser Gly Lys Gly Ser Gln
 210 215 220
 Gln Ser Val Glu Gln Ala Tyr Ala Glu Ala Gly Gln Pro Gln His Lys
 225 230 235 240
 Val Thr Glu Phe Ile Asp Asp Met Ala Ala Ala Tyr Ala Trp Ala Asp
 245 250 255
 Val Val Val Cys Arg Ser Gly Ala Leu Thr Val Ser Glu Ile Ala Ala
 260 265 270
 Ala Gly Leu Pro Ala Leu Phe Val Pro Phe Gln His Lys Asp Arg Gln
 275 280 285
 Gln Tyr Trp Asn Ala Leu Pro Leu Glu Lys Ala Gly Ala Ala Lys Ile
 290 295 300
 Ile Glu Gln Pro Gln Leu Ser Val Asp Ala Val Ala Asn Thr Leu Ala
 305 310 315 320
 Gly Trp Ser Arg Glu Thr Leu Leu Thr Met Ala Glu Arg Ala Arg Ala
 325 330 335
 Ala Ser Ile Pro Asp Ala Thr Glu Arg Val Ala Asn Glu Val Ser Arg
 340 345 350
 Val Ala Arg Ala Leu Glu His His His His His His
 355 360

<210> 2

<211> 351

<212> PRT

<213> Haemophilus influenzae

<400> 2

Met Lys Asn Lys Lys Leu Leu Val Met Ala Gly Gly Thr Gly Gly His
 1 5 10 15

Val Phe Pro Ala Ile Ala Val Ala Gln Thr Leu Gln Lys Gln Glu Trp
 20 25 30

Asp Ile Cys Trp Leu Gly Thr Lys Asp Arg Met Glu Ala Gln Leu Val
 35 40 45

Pro	Lys	Tyr	Gly	Ile	Pro	Ile	Arg	Phe	Ile	Gln	Ile	Ser	Gly	Leu	Arg	50	55	60
Gly	Lys	Gly	Ile	Lys	Ala	Leu	Leu	Asn	Ala	Pro	Phe	Ala	Ile	Phe	Arg	65	70	75
Ala	Val	Leu	Gln	Ala	Lys	Lys	Ile	Ile	Gln	Glu	Glu	Lys	Pro	Asp	Ala	85	90	95
Val	Leu	Gly	Met	Gly	Gly	Tyr	Val	Ser	Gly	Pro	Ala	Gly	Val	Ala	Ala	100	105	110
Lys	Leu	Cys	Gly	Val	Pro	Ile	Ile	Leu	His	Glu	Gln	Asn	Ala	Ile	Ala	115	120	125
Gly	Leu	Thr	Asn	Lys	Leu	Leu	Gly	Lys	Ile	Ala	Thr	Cys	Val	Leu	Gln	130	135	140
Ala	Phe	Pro	Thr	Ala	Phe	Pro	Met	Ala	Glu	Val	Val	Gly	Asn	Pro	Val	145	150	155
Arg	Glu	Asp	Leu	Phe	Glu	Met	Pro	Asn	Pro	Asp	Ile	Arg	Phe	Ser	Asp	165	170	175
Arg	Glu	Glu	Lys	Leu	Arg	Val	Leu	Val	Val	Gly	Gly	Ser	Gln	Gly	Ala	180	185	190
Arg	Val	Leu	Asn	His	Thr	Leu	Pro	Lys	Val	Val	Ala	Gln	Leu	Ala	Asp	195	200	205
Lys	Leu	Glu	Phe	Arg	His	Gln	Val	Gly	Lys	Gly	Ala	Val	Glu	Glu	Val	210	215	220
Ser	Gln	Leu	Tyr	Gly	Glu	Asn	Leu	Glu	Gln	Val	Lys	Ile	Thr	Glu	Phe	225	230	235
Ile	Asp	Asn	Met	Ala	Glu	Ala	Tyr	Ala	Trp	Ala	Asp	Val	Val	Ile	Cys	245	250	255
Arg	Ser	Gly	Ala	Leu	Thr	Val	Cys	Glu	Ile	Ala	Ala	Val	Gly	Ala	Ala	260	265	270
Ala	Ile	Phe	Val	Pro	Phe	Gln	His	Lys	Asp	Arg	Gln	Gln	Tyr	Leu	Asn	275	280	285
Ala	Lys	Tyr	Leu	Ser	Asp	Val	Gly	Ala	Ala	Lys	Ile	Ile	Glu	Gln	Ala	290	295	300
Asp	Leu	Thr	Pro	Glu	Ile	Leu	Val	Asn	Tyr	Leu	Lys	Asn	Leu	Thr	Arg	305	310	315
Glu	Asn	Leu	Leu	Gln	Met	Ala	Leu	Lys	Ala	Lys	Thr	Met	Ser	Met	Pro	325	330	335
Asn	Ala	Ala	Gln	Arg	Val	Ala	Glu	Val	Ile	Lys	Gln	Tyr	Ser	Asn		340	345	350

<210> 3
 <211> 362
 <212> PRT
 <213> Enterococcus faecalis

<400> 3
 Met Lys Ile Leu Val Thr Gly Gly Gly Thr Gly Gly His Ile Tyr Pro
 1 5 10 15
 Ala Leu Ser Phe Val Glu His Val Lys Lys Glu Ala Pro Ala Thr Glu
 20 25 30

Phe Leu Tyr Val Gly Thr Glu Asn Gly Leu Glu Ser Gln Ile Val Pro
 35 40 45
 Lys Ala Lys Ile Pro Phe Lys Thr Ile Lys Ile Gln Gly Phe Lys Arg
 50 55 60

Ser Leu Ser Pro Gln Asn Phe Lys Thr Ile Tyr Leu Phe Leu Thr Ser
 65 70 75 80
 Ile Asn Lys Ala Lys Lys Ile Ile Arg Glu Phe Gln Pro Asp Val Val
 85 90 95

Ile Gly Thr Gly Gly Tyr Val Ser Gly Ala Val Val Tyr Ala Ala His
 100 105 110
 Gln Leu Lys Ile Pro Thr Ile Ile His Glu Gln Asn Ser Ile Pro Gly
 115 120 125

Met Thr Asn Lys Phe Leu Ser Arg Tyr Val Asp Lys Ile Ala Ile Cys
 130 135 140
 Phe Pro Asp Val Ala Ser Phe Phe Pro Lys Glu Lys Thr Ile Leu Thr
 145 150 155 160

Gly Asn Pro Arg Gly Gln Glu Val Val Thr Val Glu Lys Ser Ala Ile
 165 170 175
 Leu Ser Glu Phe Gly Leu Asp Pro Ala Lys Lys Thr Val Val Leu Phe
 180 185 190

Gly Gly Ser Arg Gly Ala Leu Lys Ile Asn Gln Ala Phe Glu Gln Ala
 195 200 205
 Phe Pro Leu Phe Glu Glu Arg Glu Tyr Gln Val Leu Tyr Ala Ser Gly
 210 215 220

Glu Arg Tyr Tyr Gln Glu Leu Gln Glu Ser Leu Lys Leu Ser Glu Lys
 225 230 235
 Lys Leu Thr Asn Ile Ser Val Gln Pro Tyr Ile Asp Lys Met Val Glu
 240 245 250

Val Met Ala Asn Thr Asp Leu Met Val Gly Arg Ala Gly Ala Thr Ser
 255 260 265 270

Ile Ala Glu Phe Thr Ala Leu Gly Leu Pro Ala Ile Leu Ile Pro Ser
 275 280 285
 Pro Tyr Val Thr Asn Asp His Gln Thr Lys Asn Ala Gln Ser Leu Val
 290 295 300
 Lys Val Gly Ala Val Glu Met Ile Pro Asp Ala Glu Leu Thr Gly Ala
 305 310 315 320
 Arg Leu Val Ala Ala Ile Asp Asp Ile Leu Leu Asn Asn Glu Lys Arg
 325 330 335
 Gln Gln Met Ala Thr Ala Ser Lys Gly Glu Arg Ile Pro Asp Ala Ser
 340 345 350
 Asp Arg Leu Tyr Gln Trp Lys Thr Leu Val
 355 360

<210> 4
 <211> 360
 <212> PRT
 <213> Enterococcus hirae

<400> 4
 Met Lys Ile Leu Val Thr Gly Gly Gly Thr Gly Gly His Ile Tyr Pro
 1 5 10 15
 Ala Leu Ala Phe Val Asn Tyr Val Lys Thr Lys Glu Pro Asn Thr Glu
 20 25 30
 Phe Met Tyr Val Gly Ala Gln Arg Gly Leu Glu Asn Lys Ile Val Pro
 35 40 45
 Glu Thr Gly Met Pro Phe Arg Thr Leu Glu Ile Gln Gly Phe Gln Arg
 50 55 60
 Lys Leu Ser Leu His Asn Leu Lys Thr Ile Gln Leu Phe Leu Lys Ser
 65 70 75 80
 Ile Arg Glu Ala Lys Lys Ile Leu Lys Glu Phe Lys Pro Asp Val Val
 85 90 95
 Ile Gly Thr Gly Gly Tyr Val Ser Gly Ala Val Val Tyr Ala Ala Ser
 100 105 110
 Lys Leu Ala Ile Pro Thr Ile Ile His Glu Gln Asn Ser Val Pro Gly
 115 120 125
 Ile Thr Asn Lys Phe Leu Ser Arg Tyr Val Asp Arg Ile Ala Leu Ser
 130 135 140
 Phe Glu Asp Ala Ala Pro Phe Phe Pro Ala Glu Lys Ser Ser Leu Ile
 145 150 155 160
 Gly Asn Pro Arg Ala Gln Glu Val Ala Asp Met Asp Lys Ser Lys Ile
 165 170 175

Leu Ala Thr Tyr Gly Leu Asp Pro Glu Lys Lys Thr Val Leu Ile Phe
 180 185 190
 Gly Gly Ser Gln Gly Ala Leu Lys Ile Asn Gln Ala Val Thr Glu Phe
 195 200 205
 Leu Met Ser Phe Asp Gln Glu Tyr Gln Val Leu Tyr Ala Ser Gly Glu
 210 215 220
 Arg Tyr Tyr Lys Asp Ile Gln Thr Lys Val Pro Ala Cys Ala Asn Val
 225 230 235 240
 Ser Ile Gln Pro Tyr Ile Asn Lys Met Ala Glu Val Met Ala Ser Ser
 245 250 255
 Asp Leu Leu Val Gly Arg Ala Gly Ala Thr Ser Ile Ala Glu Leu Thr
 260 265 270
 Ala Leu Gly Leu Pro Ala Ile Leu Ile Pro Ser Pro Tyr Val Thr Asn
 275 280 285
 Asp His Gln Thr Lys Asn Ala Met Ser Leu Val Lys Asn Asn Ala Ala
 290 295 300
 Lys Met Ile Lys Asp Asp Glu Leu Asp Gly Arg Ser Leu Lys Gln Ala
 305 310 315 320
 Ile Glu Glu Ile Met Thr Asn Asp Gln Leu Gln Lys Gln Met Ser Leu
 325 330 335
 Ala Ser Lys Gln Gln Gly Ile Pro Asp Ala Ser Glu Arg Met Tyr Glu
 340 345 350
 Leu Val Lys Ser Leu Ile Gln Lys
 355 360

<210> 5
 <211> 352
 <212> PRT
 <213> Streptococcus pneumoniae

<400> 5
 Met Lys Lys Ile Val Phe Thr Gly Gly Gly Thr Val Gly His Val Thr
 1 5 10 15
 Leu Asn Leu Leu Leu Met Pro Lys Phe Ile Glu Asp Gly Trp Glu Val
 20 25 30
 His Tyr Ile Gly Asp Lys Arg Gly Ile Glu His Gln Glu Ile Leu Lys
 35 40 45
 Ser Gly Leu Asp Val Thr Phe His Ser Ile Ala Thr Gly Lys Leu Arg
 50 55 60
 Arg Tyr Phe Ser Trp Gln Asn Met Leu Asp Val Phe Lys Val Cys Trp
 65 70 75 80

<213> Rickettsia prowazekii

<400> 6

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Met Lys Lys Ile Ile Leu Val Ala Gly Gly Ile Gly Gly His Phe Phe
 1           5           10           15

Pro Ala Val Ala Leu Gly Glu Glu Leu Ile Lys Arg Gly Tyr Ile Val
      20           25           30

His Phe Ile Thr Asp Leu Arg Cys Lys Lys Tyr Ile Asn Lys Asp Met
      35           40           45

Lys Ile Ile Phe His Ile Leu Asn Leu Lys Arg Phe Ser Asn Ile Phe
      50           55           60

Leu Phe Leu Pro Ile Leu Ser Ile Thr Phe Leu Lys Ser Ile Arg Leu
      65           70           75           80

Ile Tyr Asn Ile Lys Cys Cys Val Ile Ile Gly Phe Gly Gly Tyr Pro
      85           90           95

Val Ile Ala Pro Met Phe Ala Ala Ile Phe Leu Arg Ile Pro Ile Ile
      100           105           110

Ile His Glu Gln Asn Ser Tyr Leu Gly Lys Val Asn Lys Phe Phe Ala
      115           120           125

Arg Phe Ala Lys Lys Ile Ala Thr Ser Tyr Glu Asp Ile Lys Asn Leu
      130           135           140

Pro Glu Phe Ala Lys Ser Lys Ile Val Leu Thr Gly Gly Ile Val Arg
      145           150           155           160

Lys Asn Ile Arg Glu Leu Asp Ser Phe Met Tyr Ser Val Ser Gln His
      165           170           175

Ser Leu Thr Lys Leu Thr Gln Thr Ala Leu Thr Asn Thr Phe Asn Pro
      180           185           190

Leu Val Lys Gly Arg Asn Asp Glu Phe Ala Asn Ser Asn Ile Phe Thr
      195           200           205

Ile Phe Ile Phe Gly Gly Ser Gln Gly Ala Lys Leu Phe Ser Glu Leu
      210           215           220

Ile Pro Ala Ser Ile Lys Ile Leu Met Lys Lys Gln Pro Ser Leu Glu
      225           230           235           240

Leu Asn Ile Ile Gln Gln Ala Ala Leu Asp His Gln Val Lys Ile Lys
      245           250           255

Asp Ile Tyr Ser Lys Leu Asn Ile Thr Tyr Glu Phe Ala Glu Phe Phe
      260           265           270

Asp Asn Ile Ala Leu Gln Tyr Lys Val Ala Asn Leu Val Ile Ser Arg
      275           280           285

Ala Gly Ala Ser Thr Ile Glu Glu Leu Thr Tyr Ile Gly Leu Pro Ala
      290           295           300

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Ile Phe Ile Pro Leu Pro Ser Ala Ala Asp Asn His Gln Tyr Tyr Asn
 305 310 315 320

Ala Lys Leu Leu Glu Asp Asn Lys Ala Gly Trp Cys Leu Glu Gln Asn
 325 330 335

Asn Ile Ser Ser Glu Lys Leu Ala Asp Lys Ile Leu Asp Leu Ile Ser
 340 345 350

Asn Arg Gln Leu Leu Glu Asp Ala Ser Gln Asn Leu Leu Asn Arg Lys
 355 360 365

Lys Glu Gly His Val Leu Leu Ser Asn Leu Ile Glu Asp Thr Val Phe
 370 375 380

Leu
 385

<210> 7
 <211> 363
 <212> PRT
 <213> Bacillus subtilis

<400> 7
 Met Arg Ile Ala Ile Ser Gly Gly Gly Thr Gly Gly His Thr Tyr Pro
 1 5 10 15

Ala Leu Ala Phe Ile Lys Glu Val Gln Arg Arg His Pro Asn Val Glu
 20 25 30

Phe Leu Tyr Ile Gly Thr Glu Asn Gly Leu Glu Lys Lys Ile Val Glu
 35 40 45

Arg Glu Asn Ile Pro Phe Arg Ser Ile Glu Ile Thr Gly Phe Lys Arg
 50 55 60

Lys Leu Ser Phe Glu Asn Val Lys Ile Val Met Arg Phe Leu Lys Gly
 65 70 75 80

Val Lys Lys Ser Lys Ser Tyr Leu Ala Glu Phe Lys Pro Asp Ala Val
 85 90 95

Ile Gly Thr Gly Gly Tyr Val Cys Gly Pro Val Val Tyr Ala Ala Ala
 100 105 110

Lys Met Gly Ile Pro Thr Ile Val His Glu Gln Asn Ser Leu Pro Gly
 115 120 125

Ile Thr Asn Lys Phe Leu Ser Lys Tyr Val Asn Lys Val Ala Ile Cys
 130 135 140

Phe Glu Glu Ala Lys Ser His Phe Pro Ser Glu Lys Val Val Phe Thr
 145 150 155 160

Gly Asn Pro Arg Ala Ser Glu Val Val Ser Ile Lys Thr Gly Arg Ser
 165 170 175

Leu Ala Glu Phe Lys Leu Ser Glu Asp Lys Lys Thr Val Leu Ile Phe
 180 185 190
 Gly Gly Ser Arg Gly Ala Ala Pro Ile Asn Arg Ala Val Ile Asp Met
 195 200 205
 Gln Asp Val Leu Lys Thr Arg Asp Tyr Gln Val Leu Tyr Ile Thr Gly
 210 215 220
 Glu Val His Tyr Glu Lys Val Met Asn Glu Leu Lys Ser Lys Gly Ala
 225 230 235 240
 Ala Asp Asn Met Val Thr Lys Pro Phe Leu His Gln Met Pro Glu Tyr
 245 250 255
 Leu Lys Ala Ile Asp Val Ile Val Ala Arg Ala Gly Ala Ala Thr Ile
 260 265 270
 Ala Glu Ile Thr Ala Leu Gly Ile Pro Ser Val Leu Ile Pro Ser Pro
 275 280 285
 Tyr Val Thr Ala Asn His Gln Glu Val Asn Ala Arg Ser Leu Gly Gln
 290 295 300
 His Asp Ala Ala Ile Val Leu Lys Glu Thr Glu Leu Ser Gly Glu Lys
 305 310 315 320
 Leu Ile Glu Ala Leu Asp Arg Ile Val Leu Asn Glu Gln Thr Leu Lys
 325 330 335
 Glu Met Ser Glu Arg Thr Lys Ser Leu Gly Val Pro Asp Ala Ala Ala
 340 345 350
 Arg Leu Tyr Ser Val Leu Glu Glu Leu Lys Lys
 355 360

<210> 8
 <211> 410
 <212> PRT
 <213> Mycobacterium tuberculosis

<400> 8
 Met Lys Asp Thr Val Ser Gln Pro Ala Gly Gly Arg Gly Ala Thr Ala
 1 5 10 15
 Pro Arg Pro Ala Asp Ala Ala Ser Pro Ser Cys Gly Ser Ser Pro Ser
 20 25 30
 Ala Asp Ser Val Ser Val Val Leu Ala Gly Gly Gly Thr Ala Gly His
 35 40 45
 Val Glu Pro Ala Met Ala Val Ala Asp Ala Leu Val Ala Leu Asp Pro
 50 55 60
 Arg Val Arg Ile Thr Ala Leu Gly Thr Leu Arg Gly Leu Glu Thr Arg
 65 70 75 80

Leu Val Pro Gln Arg Gly Tyr His Leu Glu Leu Ile Thr Ala Val Pro
 85 90 95
 Met Pro Arg Lys Pro Gly Gly Asp Leu Ala Arg Leu Pro Ser Arg Val
 100 105 110
 Trp Arg Ala Val Arg Glu Ala Arg Asp Val Leu Asp Asp Val Asp Ala
 115 120 125
 Asp Val Val Val Gly Phe Gly Gly Tyr Val Ala Leu Pro Ala Tyr Leu
 130 135 140
 Ala Ala Arg Gly Leu Pro Leu Pro Pro Arg Arg Arg Arg Ile Pro
 145 150 155 160
 Val Val Ile His Glu Ala Asn Ala Arg Ala Gly Leu Ala Asn Arg Val
 165 170 175
 Gly Ala His Thr Ala Asp Arg Val Leu Ser Ala Val Pro Asp Ser Gly
 180 185 190
 Leu Arg Arg Ala Glu Val Val Gly Val Pro Val Arg Ala Ser Ile Ala
 195 200 205
 Ala Leu Asp Arg Ala Val Leu Arg Ala Glu Ala Arg Ala His Phe Gly
 210 215 220
 Phe Pro Asp Asp Ala Arg Val Leu Leu Val Phe Gly Gly Ser Gln Gly
 225 230 235 240
 Ala Val Ser Leu Asn Arg Ala Val Ser Gly Ala Ala Ala Asp Leu Ala
 245 250 255
 Ala Ala Gly Val Cys Val Leu His Ala His Gly Pro Gln Asn Val Leu
 260 265 270
 Glu Leu Arg Arg Arg Ala Gln Gly Asp Pro Pro Tyr Val Ala Val Pro
 275 280 285
 Tyr Leu Asp Arg Met Glu Leu Ala Tyr Ala Ala Ala Asp Leu Val Ile
 290 295 300
 Cys Arg Ala Gly Ala Met Ile Val Ala Glu Val Ser Ala Val Gly Leu
 305 310 315 320
 Pro Ala Ile Tyr Val Pro Leu Pro Ile Gly Asn Gly Glu Gln Arg Leu
 325 330 335
 Asn Ala Leu Pro Val Val Asn Ala Gly Gly Gly Met Val Val Ala Asp
 340 345 350
 Ala Ala Leu Thr Pro Glu Leu Val Ala Arg Gln Val Ala Gly Leu Leu
 355 360 365
 Thr Asp Pro Ala Arg Leu Ala Ala Met Thr Ala Ala Ala Ala Arg Val
 370 375 380

Gly His Arg Asp Ala Ala Gly Gln Val Ala Arg Ala Ala Leu Ala Val
385 390 395 400

Ala Thr Gly Ala Gly Ala Arg Thr Thr Thr
405 410